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# Surface reactions and adsorption on oxyhydrides

AUTHOR(S):

Tang, Ya

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酸水素化物への表面吸着と反応  
Surface reactions and adsorption on oxyhydrides

京都大学 工学研究科 物質エネルギー化学専攻 Ya Tang

研究成果概要

Heterogeneous catalytic CO<sub>2</sub> methanation is a promising CO<sub>2</sub> conversion reaction that it typically uses oxide-supported transition metals as the catalysts. For these heterogeneous catalysts, tremendous efforts have been dedicated to tuning the particle size, surface area, or cation compositions of the oxides. We have taken an oxide, barium titanate (BaTiO<sub>3</sub>) and converted it to its oxyhydride, BaTiO<sub>2.4</sub>H<sub>0.6</sub>. In the presence of Ni or Ru, the presence of hydride enhances the catalytic activity of CO<sub>2</sub> methanation by 2~7 times. We find the hydride here seems to be adequately stabilized in the perovskite oxide lattice despite the water-rich environment. Based on our kinetic analysis, we discuss the reaction mechanisms that are different from the conventional oxides and show that the lattice hydride improves the hydrogen adsorption on metal surface. However, unlike NH<sub>3</sub> synthesis, the role of hydride anion in CO<sub>2</sub> methanation reactions is still unclear. It is not trivial to gain a complete picture of the mechanism, but some simple DFT calculations offer us answers to focused questions. In other words, does the incorporation of hydride anion into BaTiO<sub>3</sub> improve the adsorption (or decrease the chemisorption energy) of CO<sub>2</sub> molecular on the oxyhydride surface?

Hence, I have been using supercomputer for the following works:

- 1/ To build the stable slab structures of BaTiO<sub>3</sub> and BaTiO<sub>3-x</sub>H<sub>x</sub> ;
- 2/ Put CO<sub>2</sub> molecular onto different oxide or oxyhydride surface and perform the DFT calculations to obtain the chemisorption energy;

$$E_{chem}^{CO_2} = E_{CO_2+slab} - E_{CO_2} - E_{slab}$$
where,  $E_{chem}^{CO_2}$  is the adsorption energy of CO<sub>2</sub> molecular,  $E_{CO_2+slab}$  is the energy of CO<sub>2</sub> and slab structures,  $E_{CO_2}$  and  $E_{slab}$  is the energy of CO<sub>2</sub> molecular and slab structure, respectively. These surface calculations are still on the way.